Absence of localization in a model with correlation measure as a random lattice

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(Received 29 October 2003; published 23 March 2004)

A coherent picture of localization in one-dimensional aperiodically ordered systems is still missing. We show the presence of purely singular continuous spectrum for a discrete system whose modulation sequence has a correlation measure which is absolutely continuous, such as for a random sequence. The system showing these properties is modeled by the Rudin-Shapiro sequence, whose correlation measure even has a uniform density. The absence of localization is also supported by a numerical investigation of the dynamics of electronic wave packets showing weakly anomalous diffusion and an extremely slow algebraic decay of the temporal autocorrelation function.

DOI: 10.1103/PhysRevB.69.094204 PACS number(s): 71.23.Ft, 63.22.+m, 73.21.Cd, 73.63.Bd

I. INTRODUCTION

The phenomenon of localization in a one-dimensional lattice in the presence of a quasiperiodic potential[1,2] has been subject to a great deal of attention over the past two decades. The motivation is to a large extent founded on the discovery of quasicrystals[3] showing long-range orientational order without being translational invariant. Another source of inspiration for studying the physical properties of structures intermediate between those of periodic and random systems is the experimental fabrication of aperiodic superlattices.[4] One of the most studied models of a one-dimensional quasicrystal is the Fibonacci lattice, which exhibits a critical behavior of localization of the eigenstates independent of the two values taken by the substitution potential. The criticality of the localization is revealed by a singular continuous energy spectrum consisting of a Cantor set of zero Lebesgue measure for the Fibonacci Hamiltonian.[5–7] This is in contrast to the behavior of models for incommensurate crystals,[8] where the potential takes values from a continuous set, which can show both localization and delocalization depending on the modulation potential.[9,10] The study of localized magnetic moments in the context of aperiodic Ising models has also been a subject of great popularity.[11]

Substitution sequences provide examples of various types of aperiodic structures, built up from a finite number of elements, which can be characterized by the nature of their Fourier spectrum. An important conceptual question is whether the spectral and transport properties of these systems depend on the correlation measures[12] of the sequences themselves. Quasiperiodic sequences have correlation measures which are pure point, but where the positions of the δ peaks are incompatible with any translational invariance. A prominent example of a substitution sequence not being quasiperiodic is given by the Thue-Morse sequence, whose correlation measure is singular continuous. However, the spectrum of a tight-binding Hamiltonian with a Thue-Morse potential is purely singular continuous,[13] and the corresponding eigenstates are again neither localized nor extended in the usual (more formal) sense. Due to a certain type of correlation in the Thue-Morse sequence, there exist states extended over the entire lattice.[14–16] It is also interesting to note that similar extended states even have been found in correlated random systems.[17] Within the class of substitutionally generable systems the Rudin-Shapiro sequence[18,19] holds a unique position inasmuch as its correlation measure is absolutely continuous,[12] such as for random sequences. Based on this feature one would expect the Rudin-Shapiro lattice to have properties close to that of a random system, especially since its correlation measure has a uniform density. However, the Rudin-Shapiro sequence has zero configurational entropy since it is deterministic in the sense that it does not admit a stochastic description. There is still no rigorous result on the absence of eigenvalues in the spectrum of a Hamiltonian with a Rudin-Shapiro potential. Quite on the contrary, extensive numerical simulations of large but finite approximations of the Rudin-Shapiro lattice have even suggested a pure point spectrum,[20,21] at least for strong enough values of the potential, exactly like what is valid for a random lattice. An analogous result has been obtained from numerical simulations of the dynamics of electronic wave packets in this lattice.[22]

The main purpose of this paper is to prove the absence of localization in a one-dimensional tight-binding model with a Rudin-Shapiro potential. This is a unique result on the absence of point spectrum of a Hamiltonian with a substitution potential whose correlation measure is absolutely continuous. This example shows that the relation between the spectrum of the Hamiltonian and the Fourier spectrum of the underlying sequence is completely lost in the sense that the gaps in the energy spectrum (which is a Cantor set of zero Lebesgue measure) constitute a dense set in spite of the absence of singularities in the Fourier spectrum. Such a relation, present for periodic and smooth enough quasiperiodic structures, seems to be limited to first-order perturbation theory.[23] This result, presented in Sec. II, strongly suggests that singular continuous energy spectrum is generic and quite independent of the correlation measures of the aperiodic sequences from the class of substitutionally generated systems.[24]

To get a more complete and coherent understanding of the physics of aperiodic order the dynamical localization properties are of fundamental importance. In Sec. III, we illustrate numerically that the dynamics of an initially localized excitation in finite approximations of the Rudin-Shapiro lattice is characterized by anomalous diffusion, which is a quite

general behavior of transport in systems with singular continuous energy spectrum. We also find the temporal autocorrelation function, which measures the time average of the probability of return, to decay algebraically in time. In contrast to the conjecture in Ref. 22, this result is in accordance with the here proven absence of a point component in its spectrum.

II. SPECTRAL CHARACTERIZATION

We will study the spectrum of the discrete Schrödinger operator H_ω, with wave functions $\psi \in l^2(\mathbb{Z})$, defined by

$$(H_\omega \psi)_n \equiv t_{n,n+1}\psi_{n+1} + t_{n,n-1}\psi_{n-1} + v(\omega_n)\psi_n . \quad (1)$$

The on-site potential $V_n \equiv v(\omega_n)$ depends on an element ω from a substitution dynamical system (Ω_u, S), where $u = (u_n)_{n\geq 0}$ represents a fixed point of a primitive substitution defined on a finite alphabet $\mathcal{A}$. Extending u to the left, using arbitrary letters from $\mathcal{A}$, giving ω, and defining Ω_u as the set of accumulation points of $\{S^n\omega | n \in \mathbb{N}\}$, where S is the left shift $(S\omega)_n = \omega_{n+1}$, makes the dynamical system (Ω_u, S) minimal and uniquely ergodic.[12] An aperiodic sequence of potentials $V_n \in \{V_A, V_B\}$ can be obtained using an injective map v from $\mathcal{A}$ to the set of real numbers $\mathbb{R}$. Nearest-neighbor hopping integrals $t_{n\pm1} \equiv t_{n,n\pm1} \in \{t_{A,A}, t_{A,B}, t_{B,A}, t_{B,B}\}$ may be assigned in correlation with the on-site potential defining a mixed tight-binding Hamiltonian.

An allowed value of the electron energy E is found from a solution of the Schrödinger equation $H_\omega \psi = E\psi$. The energy spectrum is efficiently studied by rewriting this equation in the transfer matrix formalism. Introducing $\Phi_n = (\psi_{n+1}, \psi_n)^T$ gives rise to the difference equation $\Phi_n = T_{\omega_n, t_{n\pm1}} \Phi_{n-1}$, where the transfer matrix reads

$$T_{\omega_n, t_{n\pm1}} = \begin{pmatrix} \dfrac{(E - v(\omega_n))}{t_{n,n+1}} & -\dfrac{t_{n,n-1}}{t_{n,n+1}} \\ 1 & 0 \end{pmatrix}. \quad (2)$$

For $n \geq 0$ the potentials $V_n = v(u_n)$ are to follow the Rudin-Shapiro sequence. When $V_n \in \{-1,1\}$, this sequence can be obtained from $V_0 = 1$ recursively by defining $V_{2n} = V_n$ and $V_{2n+1} = (-1)^n V_n$.[12] For an arbitrary binary distribution of letters denoted by A and B, which represent the two values V_A and V_B of the potential, the Rudin-Shapiro sequence translates into

$$u = (u_n)_{n\geq 0} = AAABAABAAAABBBABA \ldots . \quad (3)$$

This deterministic aperiodic sequence can also be generated from a substitution ξ defined by[12]

$$\xi(a) = ab, \quad \xi(b) = ac, \quad \xi(c) = db, \quad \xi(d) = dc, \quad (4)$$

acting by concatenation on the alphabet $\{a,b,c,d\}$. A final projection of the fixed point $\xi^\infty(a) \equiv \lim_{n\to\infty} \xi^n(a)$, which is obtained from an infinite application of the substitution rule (4) to the seed $\xi^0(a) \equiv a$, gives the binary sequence (3). There is, however, no one-to-one mapping between the rule (4) generating the sequence (3) and the corresponding sequence of transfer matrices given by Eq. (2). This is due to the presence of the hopping integrals $t_{A,A}$, $t_{A,B}$, $t_{B,A}$, and $t_{B,B}$ in the transfer matrices, a fact which also implies that not all of the matrices (2) belong to the group of unimodular matrices $\mathrm{SL}(2,\mathbb{R})$ on their own. This difficulty can be overcome by applying the shift $Su = (u_{n+1})_{n\geq 0}$ to Eq. (3) giving the sequence

$$Su = (u_n)_{n\geq 1} = AABAABAAAABBBABA \ldots . \quad (5)$$

This sequence cannot be obtained from the rule (4) since the uniformly continuous shift S is not one to one here. Recently, we studied[25] the possibility of transforming certain mixed tight-binding lattices to on-site models on renormalized lattices, where suitable chosen unimodular blocks of transfer matrices are renormalizable with respect to the substitution potential. It was found that the matrix relation $T_{Su} = \cdots T_{u_4} T_{u_3} T_{u_2} T_{u_1}$, where the hopping dependence of each matrix (2) is suppressed, can be represented as a dynamical system on $\mathrm{SL}(2,\mathbb{R})$ in one-to-one correspondence with a substitution generating the sequence (5). The spectral character thus remains invariant compared to the case where $t_{n,n\pm1} = 1$ in the transfer matrix (2) for all n. For negative n the matrix relation can then be written as $T_{(\omega_n)_{n\leq 0}} = \cdots T^{-1}_{\omega_{-3}} T^{-1}_{\omega_{-2}} T^{-1}_{\omega_{-1}} T^{-1}_{\omega_0}$.

Without loss of generality, we study the spectrum of the Hamiltonian (1) with all the hopping matrix elements $t_{n,n\pm1} = 1$. The dynamical system on the level of the transfer matrices is now trivially inherited from the one generated by the substitution rule at hand. Guided by the result in Ref. 25, we infer the substitution

$$\begin{aligned} &\sigma(a) = ab, \quad \sigma(b) = cd, \\ &\sigma(c) = ae, \quad \sigma(e) = cg, \\ &\sigma(f) = hd, \quad \sigma(d) = fb, \\ &\sigma(h) = hg, \quad \sigma(g) = fe, \end{aligned} \quad (6)$$

defined on the alphabet $\mathcal{A} = \{a,b,c,d,e,f,g,h\}$. This substitution has the fixed point $\sigma^\infty(a) \equiv \lim_{n\to\infty} \sigma^n(a)$ from which one can obtain the sequence (5) using the projection $v(a) = v(b) = v(d) = v(f) = V_A$, $v(c) = v(e) = v(g) = v(h) = V_B$. Another obvious choice of projection offers the possibility of obtaining also the Rudin-Shapiro sequence (3). Both the sequence u in Eq. (3) and its translated version Su in Eq. (5) are thus contained in some element $\omega \in \Omega_{\sigma^\infty(a)}$ using suitable projections. By minimality of the dynamical system, the spectrum of H_ω is the same for all nonperiodic $\omega \in \Omega_{\sigma^\infty(a)}$. Due to the absence of an absolutely continuous spectrum,[26,27] the spectral classification reduces to the distinction between point spectrum and singular continuous spectrum. Moreover, the spectrum is a Cantor set of zero Lebesgue measure[28] since the substitution (6) is primitive. However, the absence of isolated points of a Cantor set does not imply the absence of eigenvalues in the spectrum.

For the exclusion of point spectrum, we consider another dynamical system based on the traces of the transfer matrices. Given a primitive substitution on an alphabet $\mathcal{A}$, there is

a trace map over a set of words $\mathcal{B}\subset\mathcal{A}^*$, where $\mathcal{A}^*$ is the set of words on $\mathcal{A}$. To the trace map one can associate a reduced trace map,[29] being a monomial, and to this map a substitution on $\mathcal{B}$. This induced substitution can be chosen to be semiprimitive,[30] which means that there is a set $\mathcal{C}\subset\mathcal{B}$ such that the induced substitution is primitive when restricted to the set $\mathcal{C}$.[29] The authors of Ref. 30 also removed the hypothesis of the existence of a square word, which was needed in Ref. 29 to assure a singular spectrum, and showed that the spectrum indeed is a Cantor set. Here we can choose the set $\mathcal{C}=\{\sigma^2(a),\sigma^2(b),\sigma^2(g),\sigma^2(h)\}\subset\mathcal{B}$, where $\mathcal{B}$ is defined from a set of trace coordinates, some of which are $a_m^{(n)}=\mathrm{tr}\,T_{\sigma^{n+m}(a)}$, $b_m^{(n)}=\mathrm{tr}\,T_{\sigma^{n+m}(b)}$, $g_m^{(n)}=\mathrm{tr}\,T_{\sigma^{n+m}(g)}$, and $h_m^{(n)}=\mathrm{tr}\,T_{\sigma^{n+m}(h)}$ for $0\leqslant m\leqslant 2$ and a fixed $n\geqslant 0$. Following the lines in Ref. 30, we find a reduced trace map whose induced substitution on $\mathcal{B}$ diminishes to

$$a_2^{(n+1)}=a_2^{(n)}b_2^{(n)},\quad b_2^{(n+1)}=a_2^{(n)}g_2^{(n)},$$
$$g_2^{(n+1)}=h_2^{(n)}b_2^{(n)},\quad h_2^{(n+1)}=h_2^{(n)}g_2^{(n)}, \tag{7}$$

when restricted to the set $\mathcal{C}$. This relation, defining the set $\mathcal{C}$, resembles the substitution (4), but here the order between the elements is of no importance. It is useful to define the free group $\Gamma_{\mathcal{A}}$, an extension of the free semigroup $\mathcal{A}^*$, by adding the formal inverses of the letters in $\mathcal{A}$ as generators.[31] A representation of this group on the level of the transfer matrices can be established by setting $T_{\delta^{-1}}\equiv T_\delta^{-1}$ for $\delta^{-1}\in\Gamma_{\mathcal{A}}$ together with an extension of σ to a group automorphism on $\Gamma_{\mathcal{A}}$. Using this extension of the substitution (6), we can write

$$\sigma^{n+3}(a)=\sigma^n(\gamma)\sigma^n(\gamma)\sigma^n(d^{-1}g)\sigma^{n+1}(e^{-1})\times\sigma^n(b^{-1}e)\sigma^{n+1}(d), \tag{8}$$

where $\gamma\equiv\sigma^2(a)\in\mathcal{C}$. From the observation of the existence of an element $\delta=d^{-1}g\in\Gamma_{\mathcal{A}}$ satisfying

$$\sigma^{n+2}(d^{-1}g)=\sigma^{n+1}(b^{-1}e)=\sigma^n(d^{-1}g), \tag{9}$$

the norms of the transfer matrices $T^{-1}_{\sigma^n(\delta)}$ are bounded uniformly in n. The relations (8) and (9) imply[31] the absence of eigenvalues for some $\omega\in\Omega_{\sigma^\infty(a)}$ so that, for all energies in the spectrum, no solution of the Schrödinger equation tends to zero at plus infinity. A similar result is obtained at minus infinity from extending $\sigma^\infty(a)$ by concatenation to the left giving $\omega=\varsigma^\infty(\gamma_l)\sigma^\infty(\gamma)$, where $\varsigma^\infty(\gamma_l)\equiv\lim_{n\to\infty}\sigma^{2n+2}(b)$ is a left fixed point of $\gamma_l\equiv\sigma^2(b)\in\mathcal{C}$. Now $\sigma^{2n+2}(b)=\sigma^{2n}(a)\sigma^{2n}(e)\sigma^{2n}(f)\sigma^{2n}(b)$ can be manipulated as in Eq. (8) such that it ends with a square preceded by an invariant element as in Eq. (9). This concludes the proof of the absence of point spectrum of the Hamiltonian H_ω for $t_{n,n\pm1}=1$ and some fixed ω in $\Omega_{\sigma^\infty(a)}$ there among the Rudin-Shapiro sequence (3).

Returning to the mixed Hamiltonian with the hopping matrix elements defined in correlation with the potential $v(\omega_n)$, where the sequence (5) represents the potential for $n\geqslant 1$, the spectrum remains purely singular continuous. Moreover, since this system maps onto the description of elastic vibrations in a harmonic lattice with particles having masses m_A and m_B with the same arrangement, the classical phononic spectrum is purely singular continuous.[25] One may note that neither the substitution (4) nor the Thue-Morse substitution defined by $\xi(A)=AB$ and $\xi(B)=BA$ permits an exclusion of eigenvalues using the method in Ref. 31. Along the lines described above one can, however, prove the absence of localization in mixed Thue-Morse lattices generated by the substitution rule $\tau(a)=ab$, $\tau(b)=ca$, $\tau(c)=cd$, and $\tau(d)=ac$.[25]

III. DYNAMICAL LOCALIZATION PROPERTIES

The study of the dynamical localization properties is the most appealing approach in determining the physical characteristics of singular continuous energy spectrum. The transport properties can be determined from the behavior of the time evolution of $\psi(t)=e^{-itH_\omega}\psi(0)$ for an initial state $\psi(0)=\psi_{n_0}(0)$ localized at site n_0 in the lattice. A measure of the spreading of the wave packet $\psi(t)$ is the mean-square displacement

$$\langle x^2(t)\rangle=\sum_n (n-n_0)^2|\psi_n(t)|^2, \tag{10}$$

which behaves like $t^{2\beta_2}$ in the asymptotic time regime. The scaling exponent β_2 governing the diffusion has been proved to be bounded from below, $D_1\leqslant\beta_2$, by the information dimension D_1 of the spectral measure associated with the initial state.[32,33] We have studied the time evolution of the square root of the quantity (10) by numerical integration of the time-dependent Schrödinger equation $H_\omega\psi(t)=i\dot{\psi}(t)$ for finite lattices, where N sites of type A and B are assigned different values $V_A=-V_B=V>0$ of the potential, in units of a constant hopping integral. Rigid boundary conditions are used. The dynamics of the logarithm of root-mean-square displacement for the relatively strong (compared to the hopping integral) value $V=\sqrt{2}$ of the potential arranged according to the Rudin-Shapiro sequence (3) with $N=4095$ ($n_0=2047$) is depicted in Fig. 1. Here the probability of finding the electron at either border is less then 10^{-160} minimizing boundary effects. Due to multiscaling in time, also called quantum intermittency,[34] linear fitting procedures can be difficult. The least-squares method applied to the asymptotics in Fig. 1 gives the scaling exponent $\beta_2=0.15\pm0.01$. This weakly subdiffusive ($0<\beta_2<1/2$) behavior of the dynamics is a consequence of the localization properties of the corresponding eigenstates[35] and resonance effects emerging from the class of states which supports the motion. Depending on the size N of the chosen approximant of the Rudin-Shapiro lattice, small quantitative differences in the scaling exponent β_2 can emerge, because the corresponding eigenstates can show variations in their localization properties.[36] However, the qualitative picture of an anomalous diffusion, which is characterized by a positive scaling exponent in the interval $0<\beta_2<1$ ($\beta_2=1/2$ for ordinary diffusion) is not violated. In the limit of the infinite lattice the anomalous diffusion is consistent with the singular continuous nature of the spectrum. We have studied the diffusion process for a number of

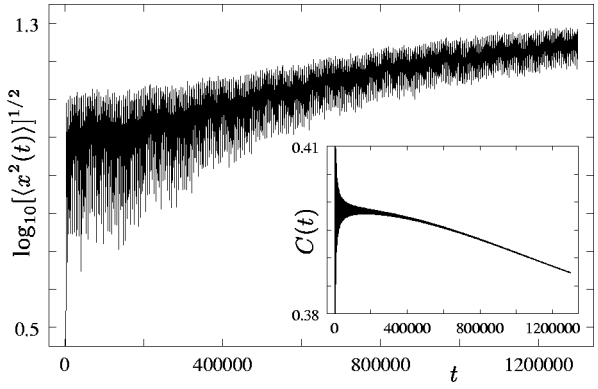

FIG. 1. The time evolution of the logarithm of the root-mean-square displacement $[\langle x^2(t)\rangle]^{1/2}$ for an electron, which at time $t=0$ was localized at site $n_0=2047$, in a lattice with $N=4095$ sites. The values $V_A=-V_B=\sqrt{2}$ of the potential are arranged according to the Rudin-Shapiro sequence (3). The inset shows the temporal autocorrelation function $C(t)$.

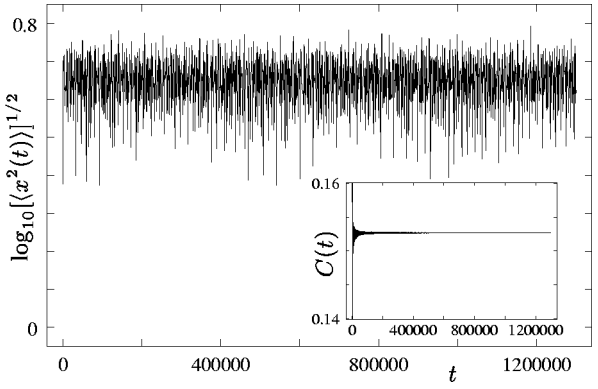

FIG. 2. Same as in Fig. 1, but for an uncorrelated random sequence with an equal fraction of elements of type *A* and *B*.

different values of the potential strength in the range $1/2 \leqslant V \leqslant 2$, and found the weakly subdiffusive dynamics to be an essentially generic behavior of the transport. Only under very special circumstances, such as for the value $V=1/\sqrt{2}$, we find superdiffusive $(1/2<\beta_2<1)$ dynamics, which is a consequence of the existence of states uniformly extended over the lattice.[37] One may notice that several hundred thousand units of time need to be considered in order to capture the asymptotic behavior in Fig. 1. In particular, the absence of diffusion $(\beta_2=0)$ found for this system in Ref. 20 is due to the fact that the time interval considered there was not long enough. Since the Rudin-Shapiro sequence shares the property of having an absolutely continuous correlation measure with random sequences, we have for comparison studied the dynamics of excitations in random lattices with the same parameter values and of the same lengths. The random lattice can be used as a reference system to the approximant of the Rudin-Shapiro lattice in order to ensure that an asymptotic region in time has been reached. We show in Fig. 2 the result corresponding to the dynamics displayed in Fig. 1, but for an uncorrelated random sequence with an equal fraction of sites of type *A* and *B*. Here the value of the scaling exponent is $\beta_2=0$, which shows the typical behavior of the absence of diffusion in an uncorrelated random lattice.

Another quantity of interest for the dynamical localization properties is the temporal autocorrelation function

$$C(t)=\frac{1}{t}\int_0^t |\psi_{n_0}(t')|^2\,dt', \tag{11}$$

which is a measure of the time average of the probability to find the electron at the initial site. In the asymptotic time limit $C(t)\sim t^{-\Delta}$, where the scaling exponent Δ ruling the algebraic decay of the averaged return probability is equal to the correlation dimension D_2.[38–40] For a random system with pure point spectrum this scaling exponent is $\Delta=0$. An example of this property can be seen in the inset of Fig. 2 for the uncorrelated random lattice. This feature is qualitatively different from what we find for the approximations of the Rudin-Shapiro lattice, which generically display very small $\Delta>0$. An illustration of this behavior is shown in the inset of Fig. 1, where an asymptotic fitting yields the scaling exponent $\Delta=0.03\pm0.01$. This numerically found algebraic decay of the temporal autocorrelation function thus supports the absence of localized eigenstates in the Rudin-Shapiro lattice from a dynamical point of view.

IV. CONCLUSIONS

In conclusion, we have rigorously proved that an absolutely continuous correlation measure of the aperiodic Rudin-Shapiro potential is not sufficient to obtain localization in one dimension. A numerical study of the dynamical localization properties of electronic wave packets in this potential revealed an anomalous diffusive behavior. Such a transport property is a rather general characteristic of singular continuous spectrum, which in turn seems to be quite independent of the nature of the correlation measure of the aperiodically ordered structure. A numerically found algebraic decay of the temporal autocorrelation function confirmed the absence of localization in the Rudin-Shapiro lattice. Finally, from an experimental point of view a Rudin-Shapiro photonic crystal could be an interesting model for slowing down light.

ACKNOWLEDGMENTS

We would like to thank Magnus Johansson for valuable discussions. Financial support from the Swedish Research Council is gratefully acknowledged.

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